

10/634,419

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \* \* \* \* \*

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DICTIONARY FILE UPDATES: 2 SEP 2005 HIGHEST RN 862457-16-7

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\*\*\*\*\*

\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*

\*\*\*\*\*

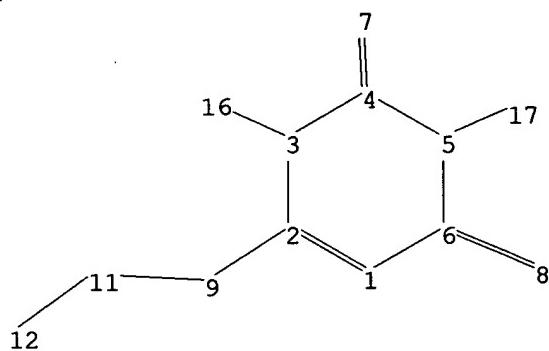
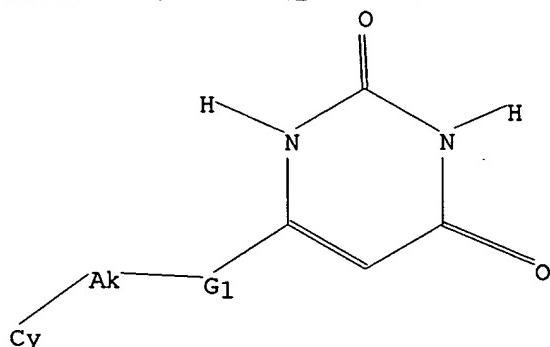
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

$\Rightarrow$

10/634, 419

Uploading C:\Documents and Settings\VBalasubramania\My Documents\STNEXP4\QUERIES\106344194.str



```
chain nodes :  
7 8 9 11 12 16 17  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
2-9 3-16 4-7 5-17 6-8 9-11 11-12  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
1-2 1-6 2-3 2-9 3-4 4-5 4-7 5-6 6-8 9-11 11-12  
exact bonds :  
3-16 5-17  
isolated ring systems :  
containing 1 :
```

G1:O, S, N

G2:H

Connectivity :  
11:2 E exact RC ring/chain  
Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS  
12:Atom 16:CLASS 17:CLASS

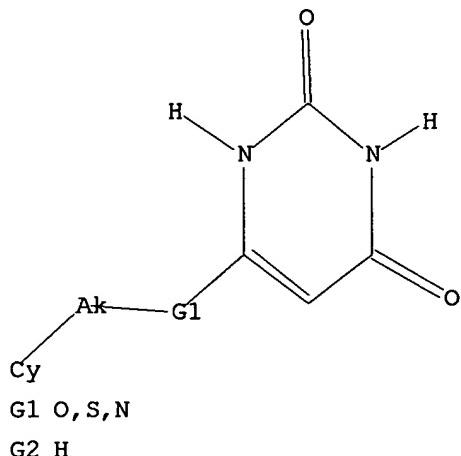
## L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

10/634,419



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 11:39:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5381 TO ITERATE

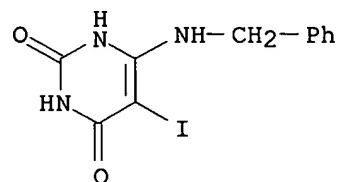
37.2% PROCESSED      2000 ITERATIONS           1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:   103222 TO   112018
PROJECTED ANSWERS:       1 TO      151

L2          1 SEA SSS SAM L1

=> d scan

L2      1 ANSWERS      REGISTRY COPYRIGHT 2005 ACS on STN
IN      2,4(1H,3H)-Pyrimidinedione, 5-iodo-6-[ (phenylmethyl)amino]- (9CI)
MF      C11 H10 I N3 O2
```



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

10/634,419

=> log y  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
0.43	0.64

STN INTERNATIONAL LOGOFF AT 11:39:34 ON 03 SEP 2005

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \*

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.scs.org/ONLINE/DBSS/registryuse.html>

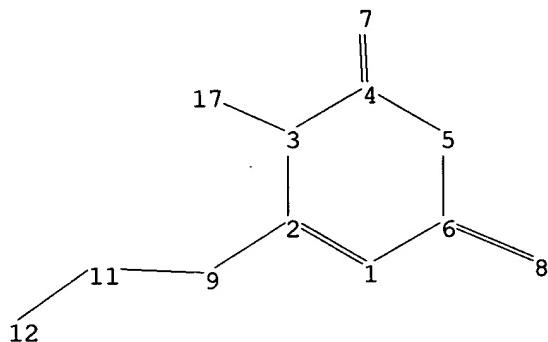
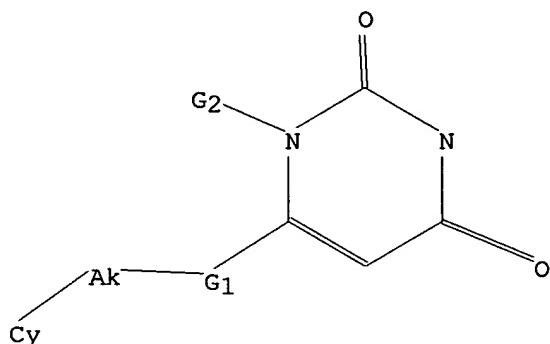
1

10/634, 419

Uploading C:\Documents and Settings\VBalasubramania\My Documents\STNEXP4\QUERIES\106344193.str

\*1

13<sup>\*1</sup>



chain nodes :

Chain nodes : 7 8 9 11 12 13 17

ring nodes :

Ring nodes .

**chain bonds :**

2-9 3-17 4-

ring bonds :

1-2    1-6    2-3    3-4

**exact/norm bonds** ...

1-2    1-6    2-3    2-9    3-4

### isolated ring system

containing 1 :

## **REFERENCES**

G1:O,S,N

G2:H, [\*1]

**Connectivity :**

11:2 E exact RC ring/chain 13:1 E exact RC ring/chain

Match level :

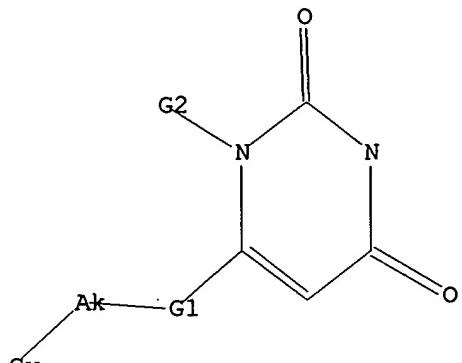
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS  
12:Atom 13:CLASS 17:CLASS

## L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

Ak<sup>1</sup>

G1 O,S,N  
G2 H,[@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam  
SAMPLE SEARCH INITIATED 11:30:52 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 5381 TO ITERATE

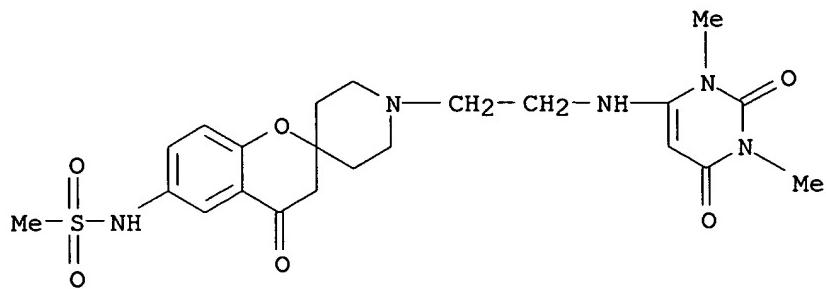
37.2% PROCESSED 2000 ITERATIONS 6 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 103222 TO 112018  
PROJECTED ANSWERS: 81 TO 563

L2 6 SEA SSS SAM L1

=> d scan

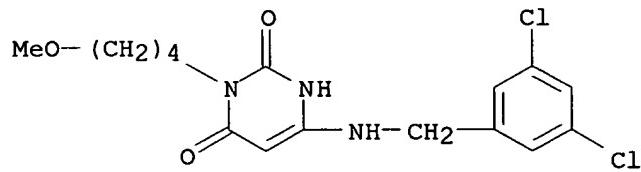
L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Methanesulfonamide, N-[3,4-dihydro-4-oxo-1'-(2-[(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)amino]ethyl]spiro[2H-1-benzopyran-2,4'-piperidin]-6-yl]- (9CI)  
MF C22 H29 N5 O6 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

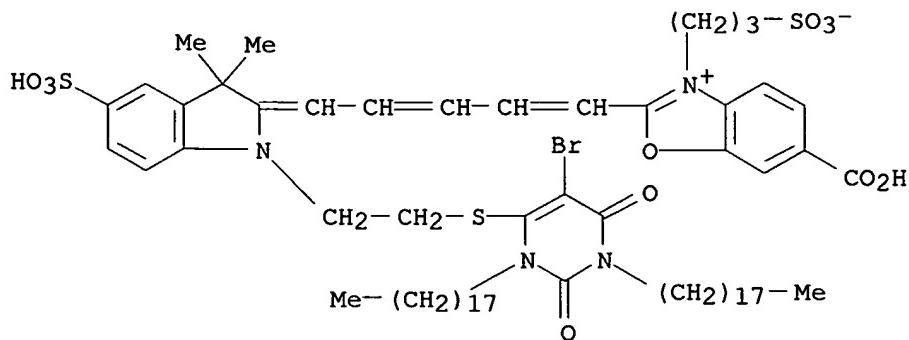
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2,4(1H,3H)-Pyrimidinedione, 6-[[[(3,5-dichlorophenyl)methyl]amino]-3-(4-methoxybutyl)- (9CI)  
MF C16 H19 Cl2 N3 O3

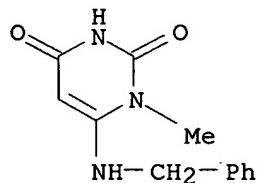


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Benzoxazolium, 2-[5-[1-[2-[(5-bromo-1,2,3,6-tetrahydro-1,3-dioctadecyl-2,6-dioxo-4-pyrimidinyl)thio]ethyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-2-ylidene]-1,3-pentadienyl]-6-carboxy-3-(3-sulfopropyl)-, inner salt (9CI)  
MF C68 H103 Br N4 O11 S3  
CI COM



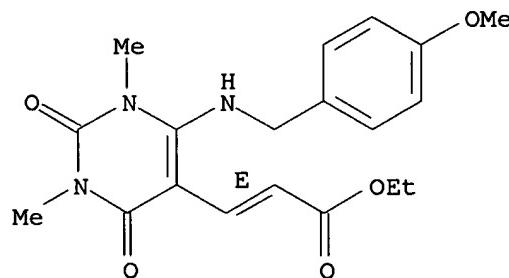
L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2,4(1H,3H)-Pyrimidinedione, 1-methyl-6-[ (phenylmethyl)amino]- (9CI)  
 MF C12 H13 N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Propenoic acid, 3-[1,2,3,4-tetrahydro-6-[(4-methoxyphenyl)methyl]amino]-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl-, ethyl ester, (E)- (9CI)  
 MF C19 H23 N3 O5

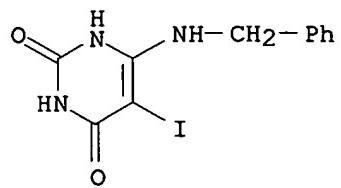
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 6 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2,4(1H,3H)-Pyrimidinedione, 5-iodo-6-[ (phenylmethyl)amino]- (9CI)  
 MF C11 H10 I N3 O2

10/634,419



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> log y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

0.86

TOTAL

SESSION

1.07

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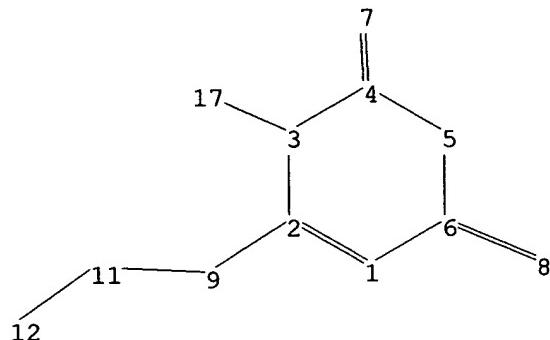
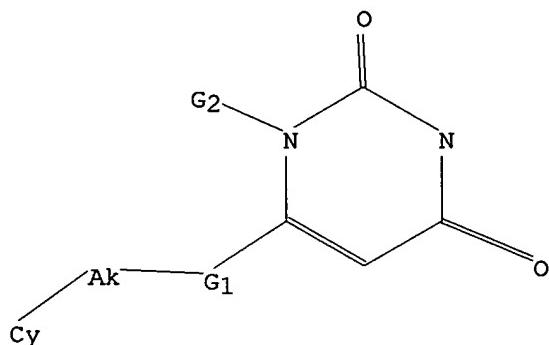
⇒

10/634,419

Uploading C:\Documents and Settings\VBalasubramania\My Documents\STNEXP4\QUERIES\106344192.str

\*1  
Ak

\*1  
13



chain nodes :

7 8 9 11 12 13 17

ring nodes :

1 2 3 4 5 6

chain bonds :

2-9 3-17 4-7 6-8 9-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 2-9 3-4 3-17 4-5 4-7 5-6 6-8 9-11 11-12

isolated ring systems :

containing 1 :

G1:O,S,N

G2:H, [\*1]

Connectivity :

13:1 E exact RC ring/chain

Match level :

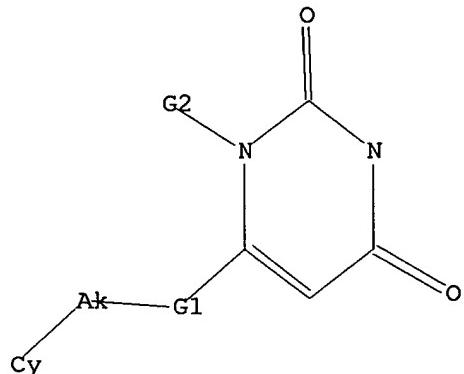
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS  
12:Atom 13:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

Ak<sup>1</sup>

G1 O, S, N  
G2 H, [@1]

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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

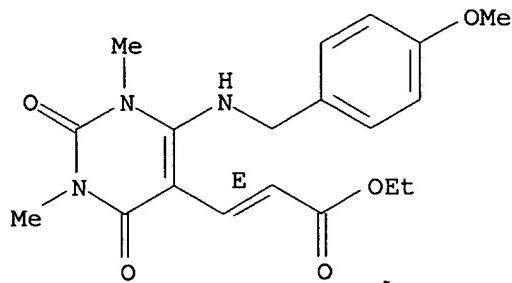
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BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 103222 TO 112018  
PROJECTED ANSWERS: 305 TO 985

L2 12 SEA SSS SAM L1

=> d scan

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2-Propenoic acid, 3-[1,2,3,4-tetrahydro-6-[(4-methoxyphenyl)methyl]amino]-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl-, ethyl ester, (E)- (9CI)  
MF C19 H23 N3 O5

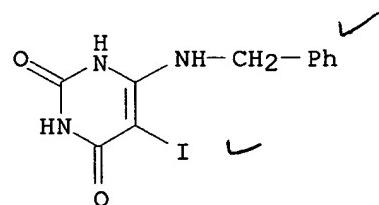
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

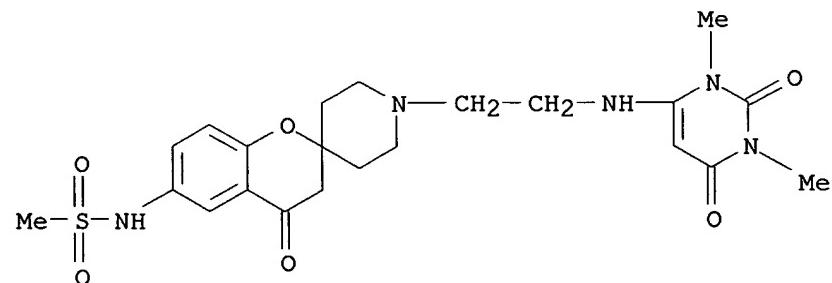
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):11

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2,4(1H,3H)-Pyrimidinedione, 5-iodo-6-[(phenylmethyl)amino]- (9CI)  
MF C11 H10 I N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

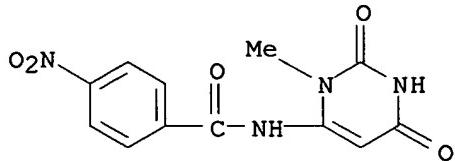
L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Methanesulfonamide, N-[3,4-dihydro-4-oxo-1'-(2-[(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)amino]ethyl]spiro[2H-1-benzopyran-2,4'-piperidin]-6-yl]- (9CI)  
MF C22 H29 N5 O6 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

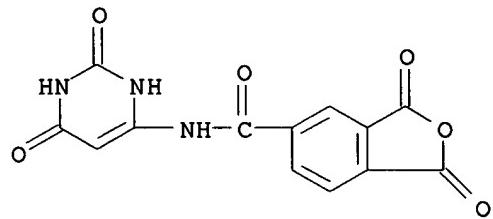
10/634,419

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Benzamide, 4-nitro-N-(1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-pyrimidinyl)-  
(9CI)  
MF C12 H10 N4 O5



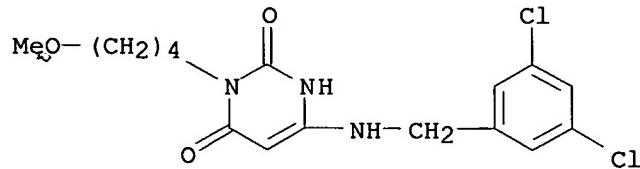
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 5-Isobenzofurancarboxamide, 1,3-dihydro-1,3-dioxo-N-(1,2,3,6-tetrahydro-  
2,6-dioxo-4-pyrimidinyl)- (9CI)  
MF C13 H7 N3 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2,4(1H,3H)-Pyrimidinedione, 6-[[[(3,5-dichlorophenyl)methyl]amino]-3-(4-  
methoxybutyl)- (9CI)  
MF C16 H19 C12 N3 O3

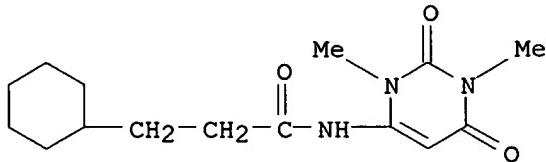


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Cyclohexanepropanamide, N-(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-

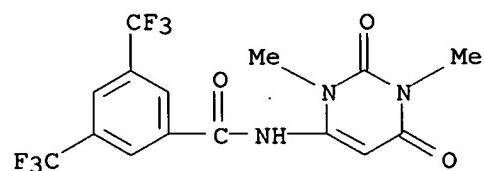
10/634,419

MF      pyrimidinyl)- (9CI)  
C15 H23 N3 O3



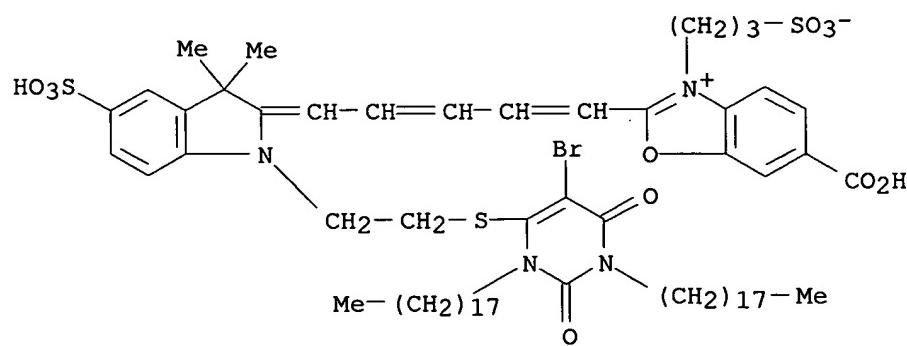
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2    12 ANSWERS    REGISTRY    COPYRIGHT 2005 ACS on STN  
IN    Benzamide, N-(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)-3,5-  
      bis(trifluoromethyl)- (9CI)  
MF    C15 H11 F6 N3 O3



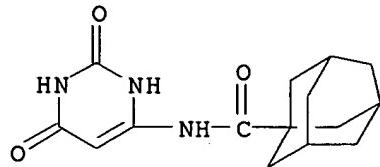
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2    12 ANSWERS    REGISTRY    COPYRIGHT 2005 ACS on STN  
IN    Benzoazolium, 2-[5-[1-[2-[(5-bromo-1,2,3,6-tetrahydro-1,3-dioctadecyl-2,6-  
dioxo-4-pyrimidinyl)thio]ethyl]-1,3-dihydro-3,3-dimethyl-5-sulfo-2H-indol-  
2-ylidene]-1,3-pentadienyl]-6-carboxy-3-(3-sulfopropyl)-, inner salt (9CI)  
MF    C68 H103 Br N4 O11 S3  
CI    COM



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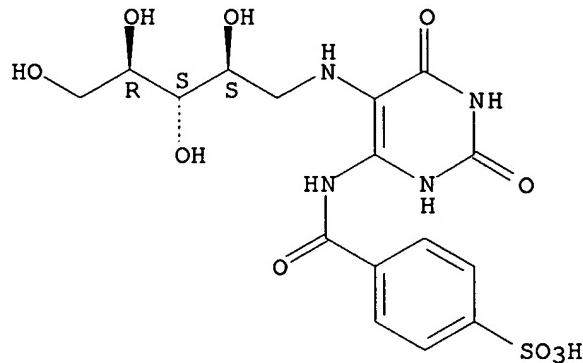
L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Tricyclo[3.3.1.13,7]decane-1-carboxamide, N-(1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinyl)- (9CI)  
MF C15 H19 N3 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

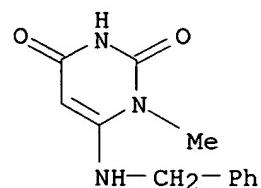
L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN D-Ribitol, 1-deoxy-1-[(1,2,3,4-tetrahydro-2,4-dioxo-6-[(4-sulfobenzoyl)amino]-5-pyrimidinyl)amino]- (9CI)  
MF C16 H20 N4 O10 S  
CI COM

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 12 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2,4(1H,3H)-Pyrimidinedione, 1-methyl-6-[(phenylmethyl)amino]- (9CI)  
MF C12 H13 N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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ALL ANSWERS HAVE BEEN SCANNED

=> log y	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.43	0.64

STN INTERNATIONAL LOGOFF AT 10:58:17 ON 03 SEP 2005